Co-Optimization of
Fuels & Engines

Fuel Property Impacts on SI Efficiency, Part 2

Project ID: FT054

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FY17 Vehicle Technologies Office
Annual Merit Review
better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Management: Kevin Stork, Gurpreet Singh, Leo Breton & Mike Weismiller

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Overview

Timeline

- Project start date: 10/1/2015
- Project end date: * 9/30/2018
- Percent complete: 60%

Budget

	FY16 Budget	FY17 Budget	FY18 Budget
VTO	$1,300k	**$1,300k**	$1,300k

Barriers

- **Complexity:** Introduction of new fuels and vehicles involves a large number of stakeholders with competing value propositions
- **Timing:** Schedule for completeing R&D and achieving market impact is extremely ambitious

Partners

Partners include 9 national laboratories, 13 universities, external advisory board, and many stakeholder and collaborators

*Start and end dates refer to three-year life cycle of DOE lab-call projects, Co-Optima is expected to extend past the end of FY18

Overview

Fuel Property Impacts on SI Efficiency Part 2

Effects of fuel properties and property quantification on engine efficiency using engine experimental data to feed into the fuel and engine Co-Optimizer.

Project	PI
Fuel Effects on EGR and Lean Dilution Limits on SI Combustion ($200k)	Kolodziej (ANL)
Studies of RON and HoV ($300k)	Kolodziej-Wallner (ANL)
Virtual CFR engine based on CFD ($200k)	Som (ANL)
Develop Optimizer Inputs ($400k)	Grout (NREL)
Co-Optimizer ($200k)	Grout (NREL)

Relevance

- Internal combustion engines will continue to dominate the fleet for decades – and their efficiency can be increased significantly.
- Research into better integration of fuels and engines is critical to accelerating progress towards our economic development, energy security, and emissions goals.
- Improved understanding in several areas is critical for progress:
    - Fuel chemistry – property relationships
    - How to measure and predict fuel properties
    - The impact of fuel properties on engine performance
- This presentation is focused on LD SI combustion. MD/HD diesel, and advanced CI combustion strategies are addressed in other Co-Optima presentations.

CI: compression ignition
HD: heavy duty
LD: light duty
MD: medium duty
SI: spark ignition

Approach

Projects have contributed to Co-Optima in two ways:

1 – Central Fuels Hypothesis

- If we correctly identify the critical fuel properties that affect efficiency and emissions performance for downsized, boosted SI engines, then fuels that have those properties will provide optimal engine performance.

2 – Boosted SI Merit Function

RON & MON (S)
Measurement & Simulation

RON & HoV

$$
\begin{aligned}
Merit = {} & \frac{(RON_{mix}-91)}{1.6} - K\frac{(S_{mix}-8)}{1.6} + \frac{0.085[ON/kJ/kg_{mix}]\cdot((HoV_{fuel}/(AFR_{stoich}+1))-(415[kJ/kg_{fuel}]/(14.3[-]+1)))}{1.6} \\
& + \frac{((HoV_{fuel}/(AFR_{stoich}+1))-(415[kJ/kg_{fuel}]/(14.3[-]+1)))}{15.38} + \frac{(S_{L\,mix}-46[cm/s])}{5.4} \\
& - H(PMI-1.6)[0.7+0.5(PMI-1.4)] + 0.008\,^{\circ}C^{-1}\left(T_{c,90,conv}-T_{c,90,mix}\right)
\end{aligned}
$$

Laminar Flame Speed

Co-Optimizer

Milestones

Tracked Milestones	Owner	Progress
Complete initial internal release of the Co-Optimizer application	Grout (NREL)	Complete (Q1)

Task Slides

Project	PI
Fuel Effects on EGR and Lean Dilution Limits on SI Combustion	Kolodziej (ANL)

Objective:

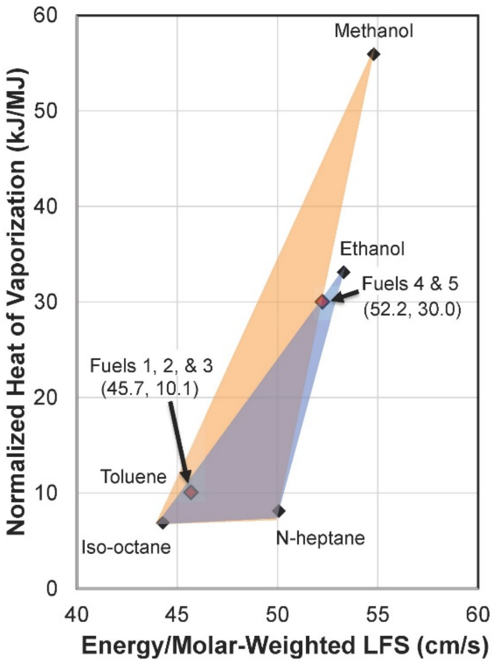
- Quantify fuel property effects on increased SI combustion lean and EGR dilution tolerance compared to engine design parameters

Approach:

- Test lean and EGR dilution limits of SI combustion with low and high laminar flame speed (LFS) pure component fuel blends

Major Outcome:

- At tested conditions, fuel LFS can extend lean and EGR dilute SI combustion by as much as engine design parameters



Component	1	2	3	4	5
iso-octane (%wt)		73.6	72.6	7.1	
n-heptane (%wt)		8.7	15.3		35.3
toluene (%wt)	100				
ethanol (%wt)		17.6		92.9	
methanol (%wt)			12.1		64.7

Task Slides

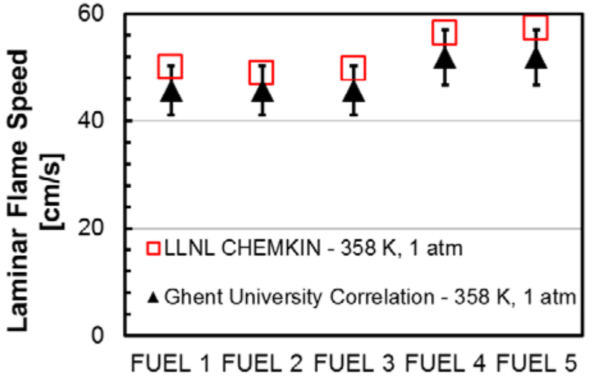
Project	PI
Fuel Effects on EGR and Lean Dilution Limits on SI Combustion	Kolodziej (ANL)

LFS Calculations:

- Ghent correlation based on Le Chatelier Rule using energy fraction

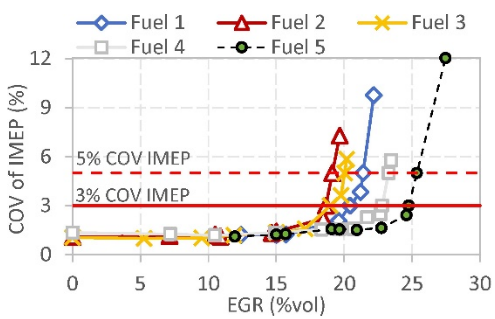
$$u_{l,\text{blend}}(\Phi) = \frac{1}{\sum_{i=1}^{n} \frac{\alpha_i}{u_{l,i}(\Phi)}}$$

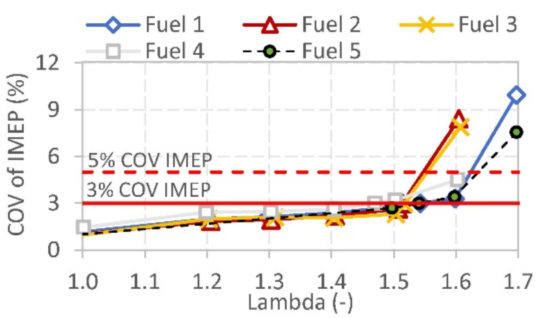
- Mixing rule compares well trend-wise with Chemkin LFS calculations



Single-Cylinder Engine Test Conditions:

- 1500 RPM, 5.6 bar $IMEP_n$
- Fixed CA50 8°aTDC
- EGR Sweep
- Lambda (Throttle) Sweep
- 0.6, 1.5 Tumble Ratio
- 75, 150 mJ Ign. Energy

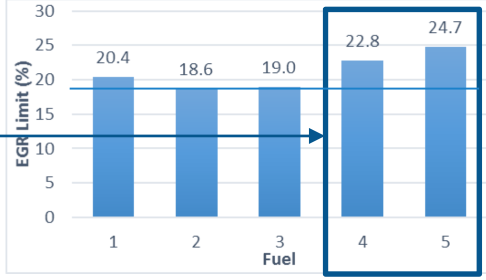


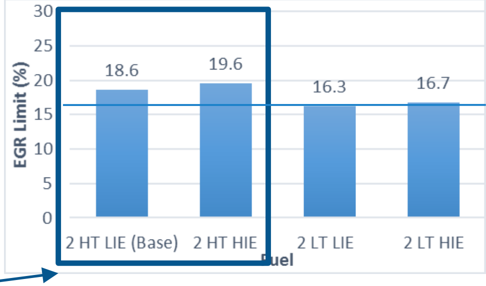


* Chemkin LFS simulations performed by Scott Wagnon and Bill Pitz, LLNL

Task Slides

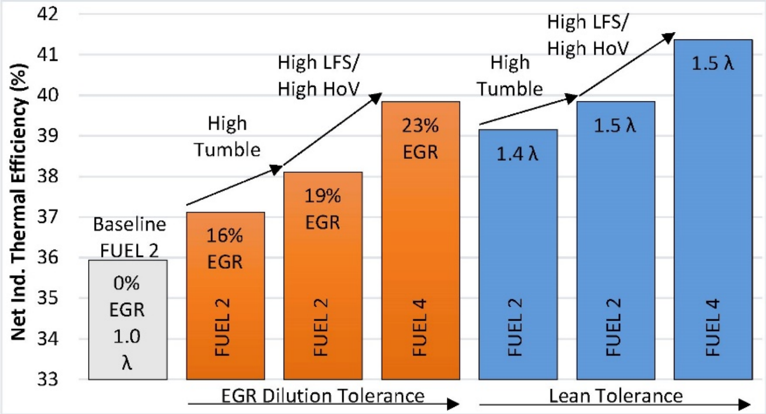
Project	PI
Fuel Effects on EGR and Lean Dilution Limits on SI Combustion	Kolodziej (ANL)





Increased dilution tolerance with higher LFS:

- Higher LFS Fuels 4/5 showed 2-5% higher EGR tolerance than Fuels 2/3
  - Fuel 1 (100% toluene) requires further research
- Higher tumble ratio (0.6→1.5) showed 2-3% higher EGR tolerance
- **Fuel LFS could extend dilution tolerance as much as engine tumble, increasing engine ITE**
- Under lean conditions, LFS did not consistently increase lean limit, but did increase ITE by 10% shorter combustion duration (2 CAD)



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Task Slides

Project	PI
Studies of RON and HoV	Kolodziej-Wallner (ANL)

Objective:

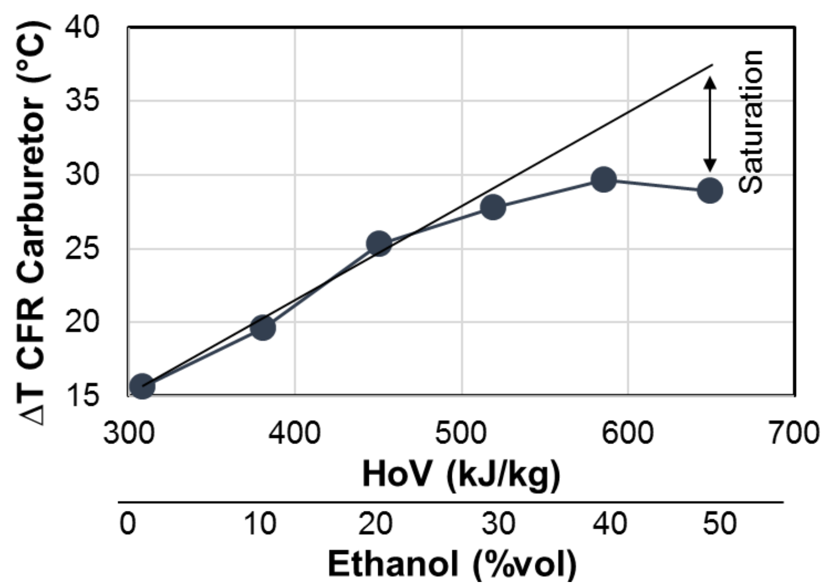
- Investigate contributions and complications of fuel property effects, especially Heat of Vaporization (HoV) on measurement of Research Octane Number (RON)

Approach:

- Characterize engine operating and combustion conditions of 98 RON fuels with varying HoV on a highly instrumented CFR engine

Major Outcome:

- Increased fuel HoV can increase RON rating of a fuel by as much as 1 ON at higher HoV levels

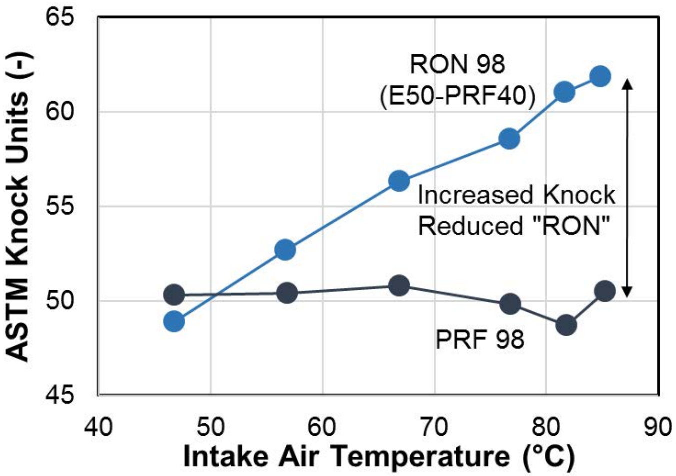


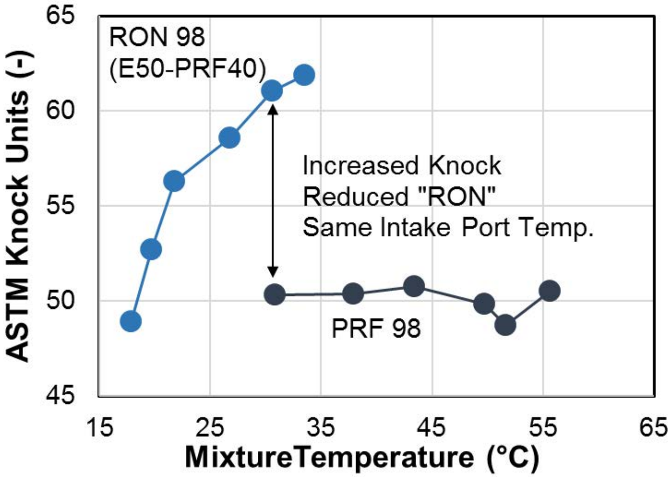
Task Slides

Project	PI
Studies of RON and HoV	Kolodziej-Wallner (ANL)

Temperature effects on RON rating:

- RON rating of ethanol-blended fuels are sensitive to changes in intake temperature
- Intake temperature cooling by increased HoV of alcohols reduces CFR knock and increases RON rating
- Intake air heating method by Foong, et al. allows common mixture temperature of high HoV fuels with PRF rating fuels
- Additional Considerations:
    - Analysis by Foong et al. used splash-blending, meaning fuel RON increased with HoV (ethanol content), necessitating higher engine CR and switching to PRF-TEL scale
    - <u>Co-Optima study uses match-blend technique at constant RON 98</u>



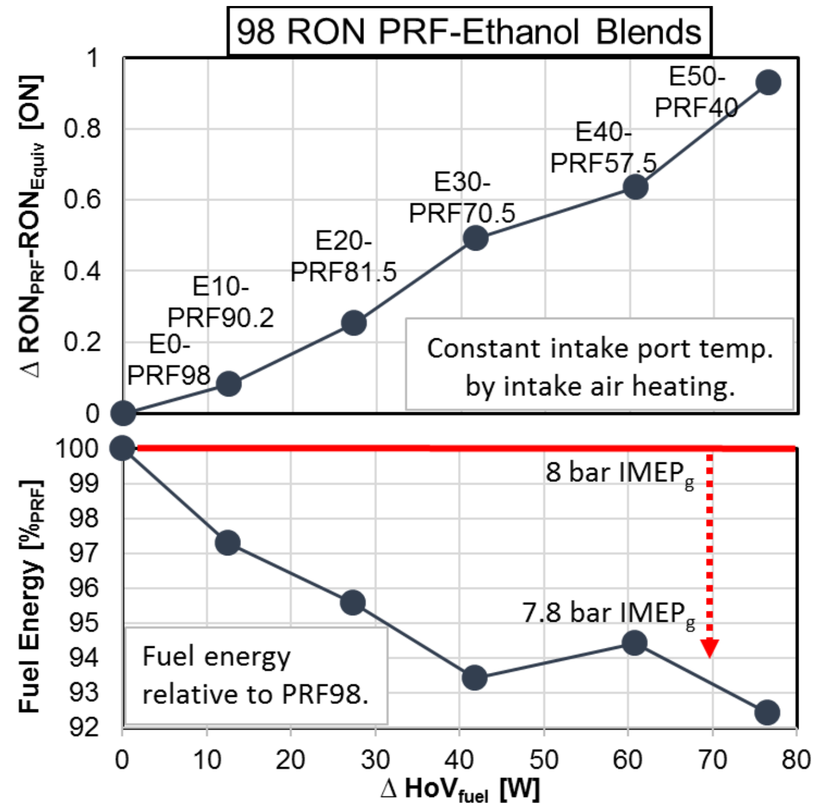


Task Slides

Project	PI
Studies of RON and HoV	Kolodziej-Wallner (ANL)

HoV contribution to RON rating:

- Several PRF-ethanol blends were match-blended with constant RON 98
- Intake air temperature (pre-carburetor) was heated above RON ASTM spec. to achieve same mixture temp. (post-carb.) as PRF rating fuels
- Increased knock was converted to reduction in "equivalent RON"
- As much 1 ON increase for E50 fuels from HoV cooling effects
- However, some measurement artifacts still need to be accounted for:
    - Decreased fuel energy rate reduces engine load
    - Slight boosting would allow for analysis at constant engine load



Task Slides

Project	PI
Virtual CFR engine based on CFD	Som (ANL)

Objective:

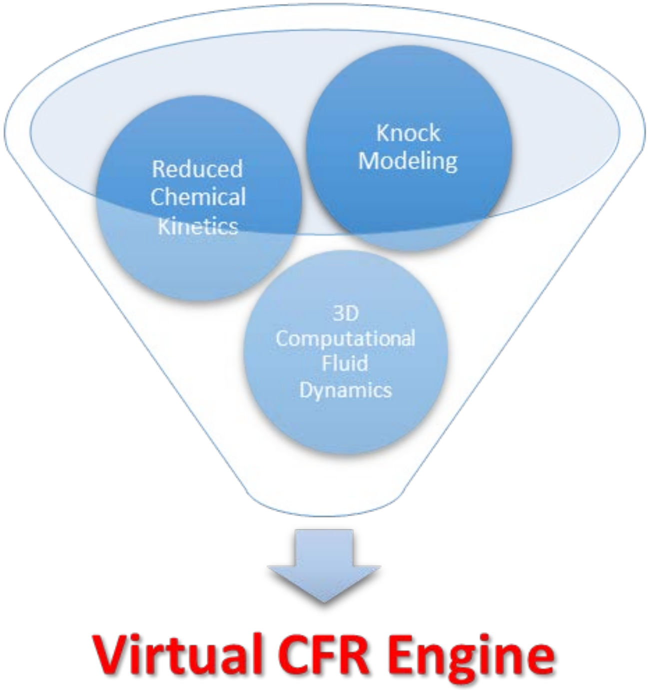
- Develop a 3D CFD modeling tool to capture knocking combustion in a CFR engine

Approach:

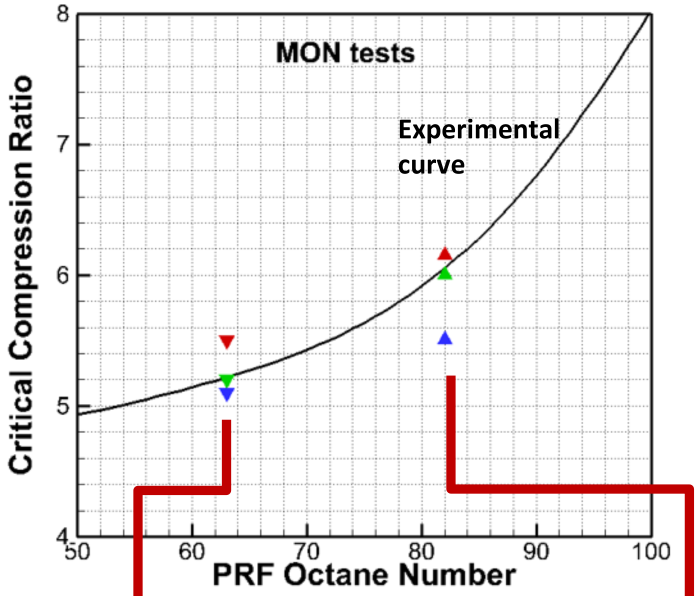
- Employ combustion modeling approaches (for both flame propagation and auto-ignition) along with reduced kinetic models for fuel chemistry to predict knock

Major Outcome:

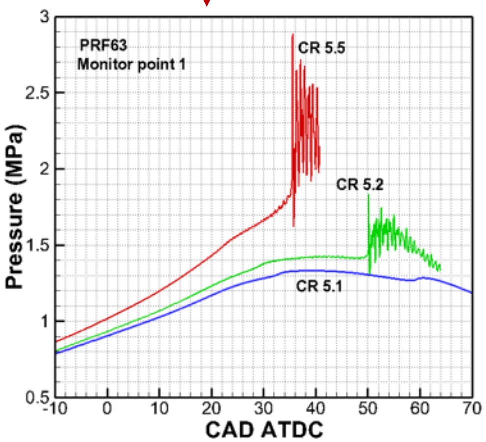
- Validation studies at RON/MON conditions show that the CFD setup can capture fuel sensitivity to knock propensity

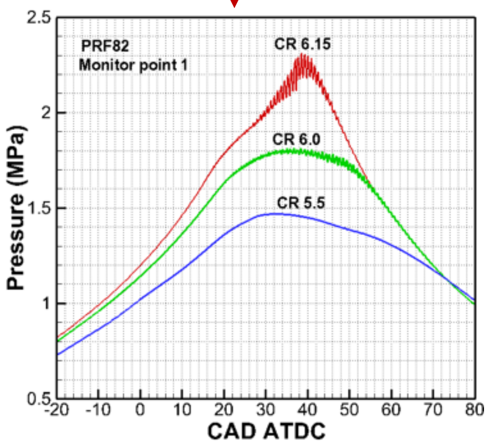


Virtual CFR Engine Based on CFD

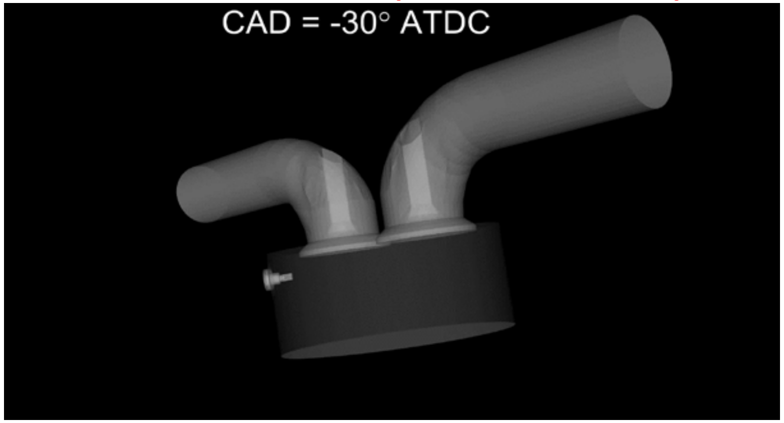


- The CFD model was validated against available experimental data at RON/MON conditions for different fuel mixtures
- The *"critical compression ratio of knock onset"* was predicted quite accurately by the RANS simulations
- The combustion and chemical kinetic models coupled with AMR were able to capture the sensitivity of knock propensity to fuel chemistry

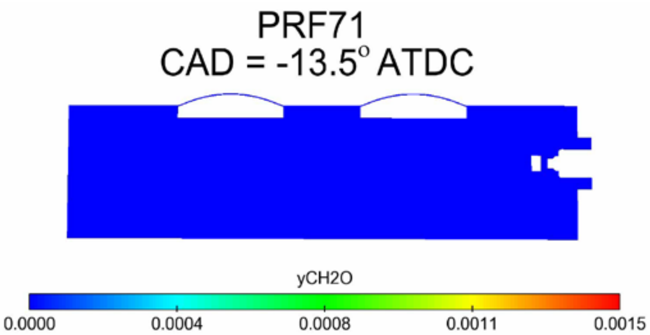


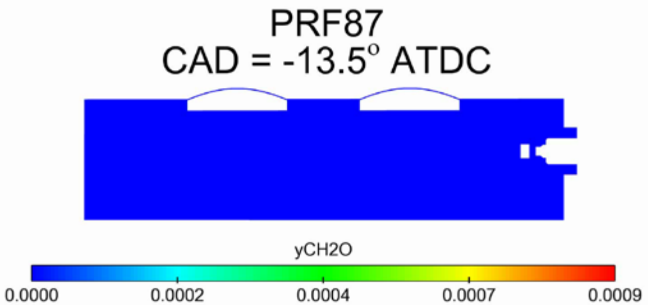


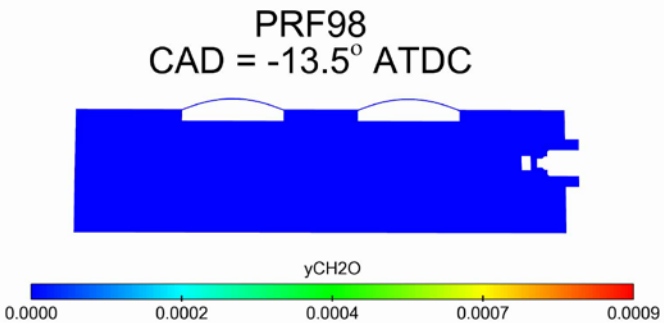
Knock visualization (PRF63 @ CR = 5.2)

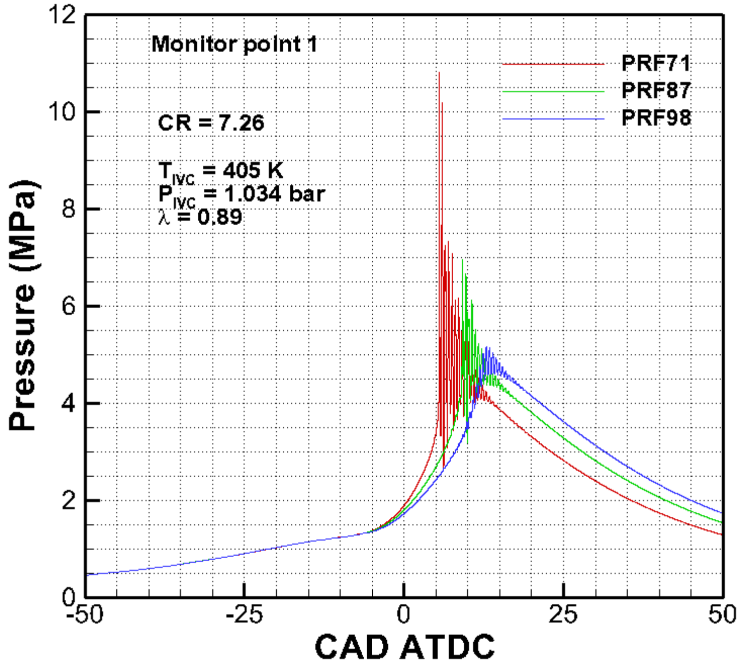


Virtual CFR Engine Based on CFD









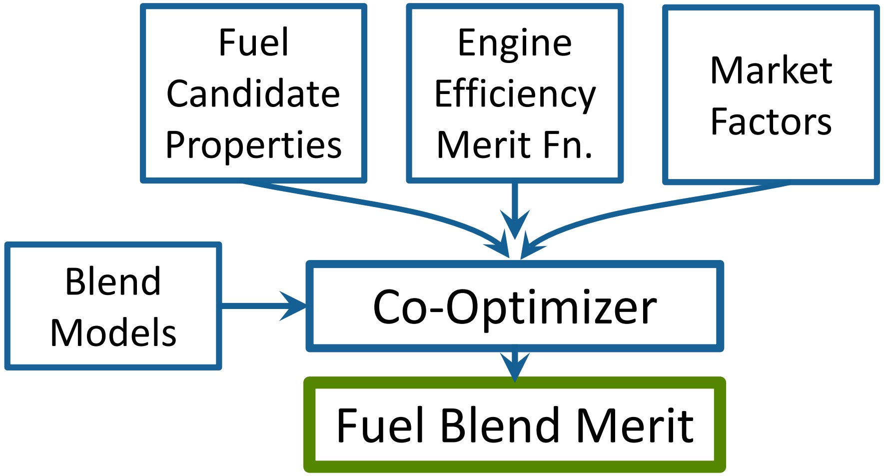
Fuel	CA50 (CAD ATDC)	Knock Onset (CAD ATDC)	Unburnt mass fraction (%) at knock onset
PRF71	5.2	4.7	56.4
PRF87	7.5	8.5	38.5
PRF98	9.4	10.0	34.2

Co-Optimizer

Project	PI
Develop Optimizer Inputs	Grout (NREL)
Co-Optimizer	Grout (NREL)

Objective:

- Integrate data from experiments, simulation, techno-economic and market factors in decision support tool, and perform scenario analysis for boosted SI fuels.
- Create capability to optimize fuel property combinations for cost function with user-defined weights for performance and cost metrics
  - e.g., MMF value, cost of production, infrastructure compatibility



Approach:

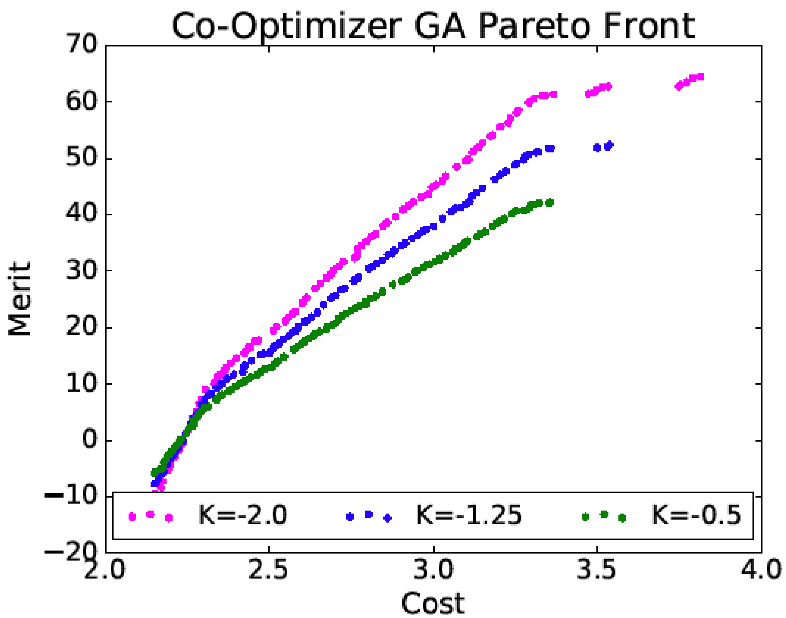
- Formulate optimization tool, use current available data and engine merit function to identify optimal fuel property combinations and sensitivities (boosted SI engines)
- Incorporate blending models to improve accuracy; make framework extensible to optimization under uncertainty.

Major Outcome:

- Stakeholders and co-optima participants will have a tool that will allow interactive exploration of the potential efficiency-cost or efficiency-value tradeoff for candidate fuels, either by mathematically rigorous fuel blend designs or ad hoc proposed blends.

Co-Optimizer

- Co-Optimizer blends components from the fuels property database to explore impact on fuel merit function
- Leverages open source tools to explore tradeoffs (cost vs. efficiency)
- Captures effect of uncertain parameters and inputs through sampling
- Implemented series of python scripts
  - Many analysis patterns implemented
  - Highly flexible
- Variety of blending models installed



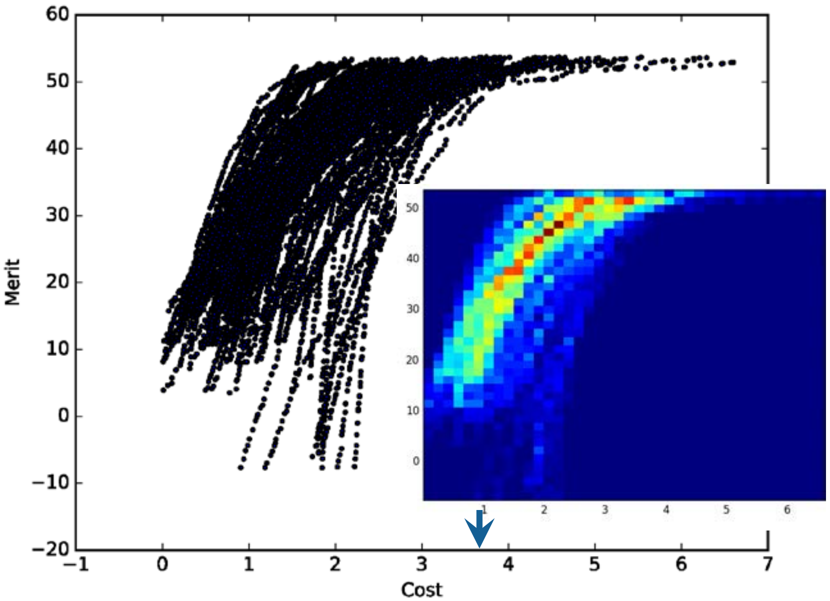
Trade-off of engine efficiency merit function against blend cost for different engine designs (K).

(Used a genetic algorithm (GA) approach to find the Pareto Front with the composition unconstrained.)

Dealing with uncertainty in cost

- Fuel component costs are user inputs due to high uncertainty
- Possible to analyze blends based on:
  - Consumer price
  - Profit margins per component
- Analysis (at right) should be taken as representative
  - User needs to specify own costs before considering the analysis in depth
  - Scatter caused by price uncertainty
- Co-optimizer can run many samples to propagate uncertainties from cost inputs to optimization results

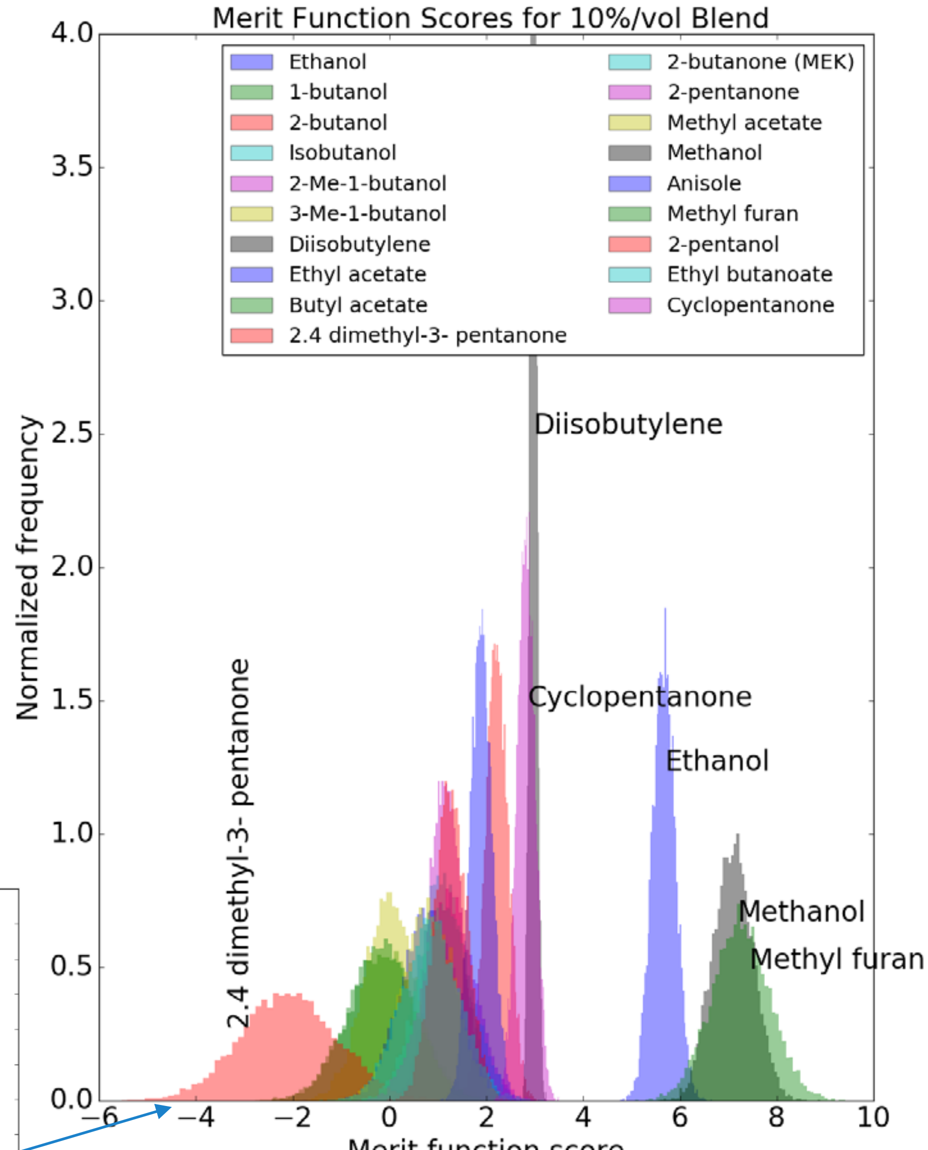
Exemplary Cost-Merit Analysis

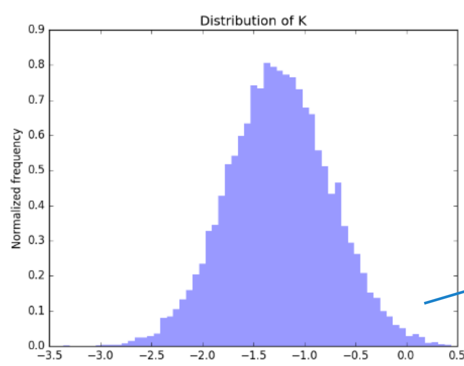


100 samples of Pareto front and corresponding density (inset) for different combinations of component costs from independent normal distributions.

Uncertainty in Merit Function Parameters

- Uncertainty propagation by sampling for fixed composition shows sensitivity of merit function to uncertainty
- Samples for K drawn from N (-1.25,0.5)
- Normalized histogram shows distribution of merit scores for each component blended at 10% by weight
- Despite scatter, clear separation for those above baseline (high merit)





Responses to 2016 AMR Reviewer Comments

Current work on laminar flame speed should be extended to other engine loads.

- The researchers agree and additional engine test conditions are being planned based on feedback from Co-Optima stakeholders.

The reviewer did not see oil company involvement.

- The task “Studies of RON and HoV” undertaken on a CFR F1/F2 engine is an example of a new project last year, which builds off of years of CFR octane rating expertise received from oil company stakeholders.

The directions of future research described are logical and potentially very useful, particularly…understanding impacts of octane sensitivity, HOV, EGR dilution tolerance, combustion flame, auto-ignition, and ultimately efficiency of high CR engines.

- In the past year, a great deal of research from several Co-Optima projects has contributed to improved understanding of the effects of these fuel properties on engine efficiency and refinement of the Boosted SI Merit Function.

Collaborations

- **Co-Optimization of Fuels and Engines** brings together expertise from across the National Laboratory system, working toward a common purpose. This effort has stakeholder engagement at a high level to ensure relevance.
  - 9 laboratories, engines, fuels, kinetics, simulation, biofuel development, LCA & TEA, market transformation
  - Monthly stakeholder engagement phone calls, industry listening days, external advisory board
- Projects presented at the semi-annual AEC program review meetings
- Engagement with ACEC Tech Team activities

Additional project-level collaborations with industry and academia:

Kolodziej

Ford – Hardware, technical guidance

Kolodziej-Wallner

Marathon Oil – Hardware, fuels, technical guidance

Som

Convergent Science – CFD code guidance

Univ. of Connecticut – Mechanism reduction

Future Work

Fuel Effects on EGR and Lean Dilution Limits on SI Combustion (Kolodziej, ANL)

- Fixed blend rate (10-30%) analysis of top Co-Optima candidate fuels into a 4-component surrogate BoB

Studies of RON and HoV (Kolodziej-Wallner, ANL)

- Test effects of BoB compositions and other high HoV Co-Optima components on RON rating and transition to saturated mixture

Virtual CFR Engine Based on CFD (Som, ANL)

- Implement 3D laser scanned geometry and verify model sensitivity for non-knocking and knocking combustion transition

Develop Co-Optimizer Inputs and Co-Optimizer (Grout, NREL)

- Explore creating <u>Co-Optimizer-based</u> engine merit function from cloud of experimental engine data and <u>improve model uncertainty analyses</u>; while improving <u>user interface</u> and accessibility

Any proposed future work is subject to change based on funding level

Summary

Relevance:

- Engine fuels and combustion experiments and simulations are necessary to improve understanding of how fuel blend characteristics can unlock increased engine efficiency
- Using this information, the Co-Optimizer, per user defined variables, is able to help analyze a vast amount of fuel property data for highest engine efficiency and fuel cost savings

Approach:

- Engine experiments and simulations provide detailed analysis on how fuel properties affect engine efficiency (fuel property hypothesis) and help to refine the Thrust 1 Merit Function, which feeds into the overall Co-Optimizer function for engine efficiency and fuel blend cost

Accomplishments:

- Fuel LFS can extend lean and EGR dilute SI combustion by as much as engine design parameters
- Increased fuel HoV can increase RON rating of a fuel by as much as 1 ON at higher HoV levels
- Validation studies at RON/MON conditions show that the CFD setup can capture fuel sensitivity to knock propensity
- A “Co-Optimizer” tool for mathematically rigorous analysis of fuel cost and engine efficiency has been developed for stakeholder and Co-Optima users

Backup Slides

Backup Slides

Project	PI
Studies of RON and HoV	Kolodziej-Wallner (ANL)

ANL instrumentation of F1/F2 CFR:

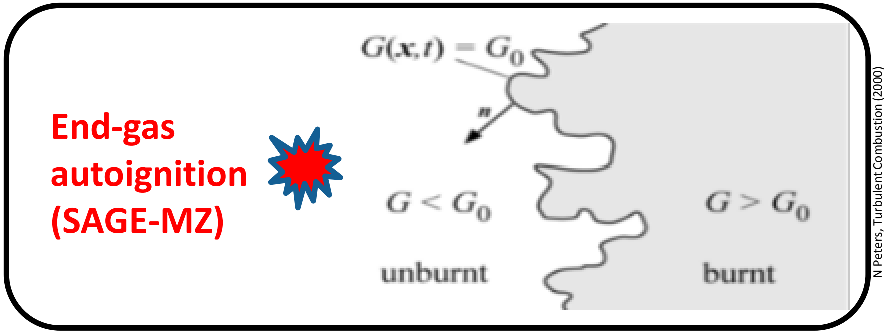
- Crank-angle resolved measurements:
  - Spark timing
  - Spark plug cylinder pressure
  - Kistler 6125C cylinder pressure in knockmeter port
  - Intake and exhaust port pressure
- Time-resolved measurements:
  - ASTM Knockmeter (digitally recorded)
  - PID controllers for RON/MON heaters
  - Relative humidity and all critical T, P
  - Fuel rate (Coriolis meter)
  - Lambda sensor
- Recent Additions:
  - Emissions/Residual Components (AVL i60 bench, FT-IR HC speciation)
  - Intake air MFC for boosted/throttled operation

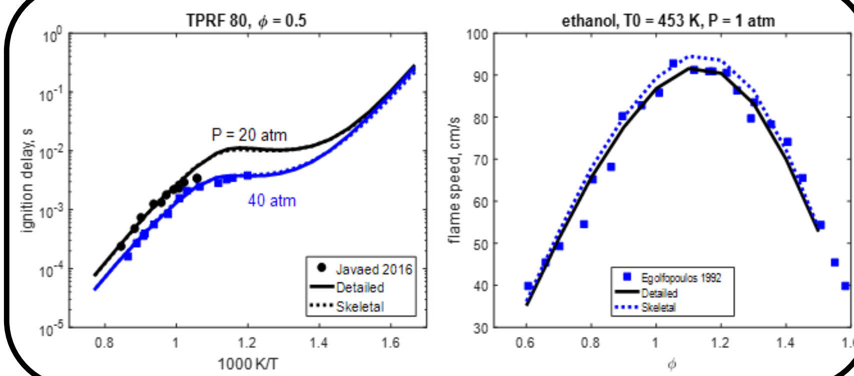
* Base CFR acquired through collaboration with Marathon Petroleum

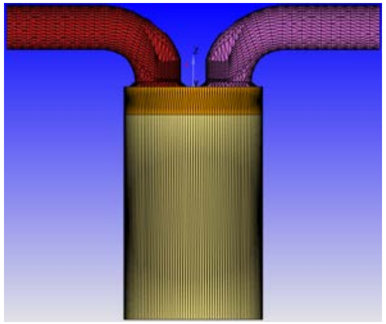
Virtual CFR Engine Based on CFD

A 3D CFD model in CONVERGE was developed to predict *knocking combustion* in a CFR engine employing:

- **Hybrid Turbulent Combustion Model** tracking flame front propagation using *"level set" approach (G-equation)* with flame speed tabulation and end-gas autoignition using *"multi-zone chemical kinetics (SAGE-MZ)"*
- **Skeletal Chemistry Mechanisms**[1] developed and validated for gasoline and gasoline/ethanol surrogate blends & suitable for CFD applications
- High-fidelity *numerical methods* & *adaptive mesh refinement (AMR)*
- Nominal *CFR engine geometry*[2]







Engine specifications and operating conditions	
Stroke	114.3 mm
Bore	82.55 mm
Connecting rod	254 mm
Engine speed	600 rpm (RON), 900 rpm (MON)
Spark timing	13^0 BTDC (RON) $19\text{-}26^0$ BTDC (MON)

[1]Mechanism reduction performed by Yunchao Wu and Prof. Tianfeng Lu at UConn
[2]Provided by Dr. Ben Wolk (SNL) and Prof. J.Y. Chen (UCB)